

Responses of small quantum systems subjected to finite baths

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Abstract

We have studied responses to applied external forces of the quantum ($N_S + N_B$) model for N_S -body interacting harmonic oscillator (HO) system subjected to N_B -body HO bath, by using canonical transformations combined with Husimi's method for a driven quantum HO [K. Husimi, Prog. Theor. Phys. **9**, 381 (1953)]. It has been shown that the response to a uniform force expressed by the Hamiltonian: $H_f = -f(t) \sum_{k=1}^{N_S} Q_k$ is generally not proportional to N_S except for no system-bath couplings, where $f(t)$ expresses its time dependence and Q_k denotes a position operator of k th particle of the system. We have calculated also the response to a space- and time-dependent force expressed by $H_f = -f(t) \sum_{k=1}^{N_S} Q_k e^{i2\pi k u/N_S}$, where the wavevector u is $u = 0$ and $u = -N_S/2$ for uniform and staggered forces, respectively. The spatial correlation Γ_m for a pair of positions of Q_k and Q_{k+m} has been studied as functions of N_S and the temperature. Our calculations have indicated an importance of taking account of finite N_S in studying quantum open systems which generally include arbitrary numbers of particles.

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I. INTRODUCTION

In recent years, there has been considerable interest in open small systems, whose physical properties have been studied both by experimental and theoretical methods [1]. We may prepare desired small systems by advanced new techniques. Theoretical studies of open systems have been made with the use of the Caldeira-Leggett (CL) type models [2–6]. CL-type models have been extensively studied by using various methods such as quantum Langevin equation and master equation [6]. The original CL model considers a system of a single particle ($N_S = 1$) which is subjected to a bath consisting of infinite numbers of uncoupled harmonic oscillators (HOs) ($N_B = \infty$). Recent studies with the CL model have tried to go beyond this restriction on N_S and N_B . References [7–9] have employed the CL model with $N_S = 1$ and $N_B \simeq 1 - 800$ for studies of properties of small system coupled to finite bath. CL-type models with $N_S = 2$ and $N_B = \infty$ have been investigated [10, 11]. Reference [12] discusses the master equation of arbitrary N_S system coupled to an arbitrary N_B bath. In our previous study [13], we have adopted the $(N_S + N_B)$ model for N_S -body system subjected to N_B -body bath in order to calculate energy distributions of a system, which show intriguing properties as functions of N_S , N_B and a system-bath coupling.

In adopting the CL-type model, we have implicitly assumed that physical quantities such as the energy and specific heat of a system with finite N_S (> 1) are given as N_S times of results of a system with $N_S = 1$. Our recent calculation [14], however, has pointed out that it is generally not the case because the system specific heat, $C_S(T; N_S, N_B)$, of the $(N_S + N_B)$ model at temperature T is given by

$$C_S(T; N_S, N_B) \neq N_S C_S(T; 1, N_B), \quad (1)$$

except for no system-bath couplings and/or in the high-temperature limit. Furthermore it has been shown that the low-temperature specific heat may be negative for finite N_S with a strong system-bath coupling [14]. This is in contrast with Refs. [15, 16, 18] showing a non-negative system specific heat for HO system in CL-type models with $(N_S, N_B) = (1, 1)$ and $(1, \infty)$. These results imply that we should explicitly take into account finite N_S in studying open systems which may generally include arbitrary numbers of particles. It is interesting and necessary to study responses to applied external forces of the $(N_S + N_B)$ model, which is the purpose of the present paper. Responses of the CL models have been

mostly made for infinite baths for which Ohmic and Drude models are adopted (*e.g.*, Ref. [19]) [6]. In this study, we employ the identical-frequency model for finite baths [14].

The paper is organized as follows. In Sec. II, we briefly explain the $(N_S + N_B)$ model [13, 14], to which we apply the canonical transformations in order to obtain the diagonalized Hamiltonian including external forces. By using Husimi's method for a driven quantum HO [21], we calculate the response of the open HO system to sinusoidal and step forces. In Sec. III, we calculate also the response to space- and time-dependent forces. The spatial correlation Γ_m between positions of two particles separated by a distance m is evaluated. The final Sec. IV is devoted to our conclusion.

II. THE $(N_S + N_B)$ MODEL

A. Quantum Langevin equation

We consider the $(N_S + N_B)$ model in which the a one-dimensional N_S -body system (H_S) is subjected to an N_B -body bath (H_B) by the interaction (H_I) [13, 14]. The total Hamiltonian is assumed to be given by

$$H = H_S + H_B + H_I, \quad (2)$$

with

$$H_S = \sum_{k=1}^{N_S} \left[\frac{P_k^2}{2M} + \frac{DQ_k^2}{2} + \frac{K}{2}(Q_k - Q_{k+1})^2 \right] + H_f, \quad (3)$$

$$H_f = -f(t) \sum_{k=1}^{N_S} Q_k, \quad (4)$$

$$H_B = \sum_{n=1}^{N_B} \left(\frac{p_n^2}{2m} + \frac{m\omega_n^2 q_n^2}{2} \right), \quad (5)$$

$$H_I = \sum_{k=1}^{N_S} \sum_{n=1}^{N_B} \frac{c_{kn}}{2} (Q_k - q_n)^2. \quad (6)$$

Here P_k (p_n) and Q_k (q_n) express the momentum and position operators, respectively, of a HO with a mass of M (m) in the system (bath), D and K denote force constants in the system, ω_n is the oscillator frequency of the bath, c_{kn} is a system-bath coupling and $f(t)$ stands for an applied force. Operators satisfy commutation relations,

$$[Q_k, P_\ell] = i\hbar\delta_{k\ell}, \quad [q_n, p_m] = i\hbar\delta_{nm}, \quad [Q_k, Q_\ell] = [P_k, P_\ell] = [q_n, q_m] = [p_n, p_m] = 0. \quad (7)$$

Equation (3) expresses the interacting HO system for $D \neq 0$ and $K \neq 0$. In the limiting case of $K = 0$, the system consists of a collection of uncoupled (independent) HOs. The system is subjected to a bath consisting of a collection of uncoupled HOs with oscillator frequencies of $\{\omega_n\}$.

In conventional approaches to the quantum system-plus-bath model, we obtain equations of motion for Q_k and q_n , employing the Heisenberg equation,

$$i\hbar\dot{O} = [O, H], \quad (8)$$

where O expresses an arbitrary operator and a dot stands for a derivative with respect of time. We obtain the quantum Langevin equations given by [14]

$$\begin{aligned} M\ddot{Q}_k(t) &= -DQ_k(t) - K[2Q_k(t) - Q_{k-1}(t) - Q_{k+1}(t)] - M \sum_{\ell=1}^{N_S} \xi_{k\ell} Q_\ell(t) \\ &\quad - \sum_{\ell=1}^{N_S} \int_0^t \gamma_{k\ell}(t-t') \dot{Q}_\ell(t') dt' - \sum_{\ell=1}^{N_S} \gamma_{k\ell}(t) Q_\ell(0) + \zeta_k(t) + f(t), \end{aligned} \quad (9)$$

with

$$M\xi_{k\ell} = \sum_{n=1}^{N_B} \left(c_{kn} \delta_{k\ell} - \frac{c_{kn} c_{\ell n}}{m\tilde{\omega}_n^2} \right), \quad (10)$$

$$\gamma_{k\ell}(t) = \sum_{n=1}^{N_B} \left(\frac{c_{kn} c_{\ell n}}{m\tilde{\omega}_n^2} \right) \cos \tilde{\omega}_n t, \quad (11)$$

$$\zeta_k(t) = \sum_{n=1}^{N_B} c_{kn} \left(q_n(0) \cos \tilde{\omega}_n t + \frac{\dot{q}_n(0)}{\tilde{\omega}_n} \sin \tilde{\omega}_n t \right). \quad (12)$$

Here $\xi_{k\ell}$ denotes the additional interaction between k and ℓ th particles in the system induced by couplings $\{c_{kn}\}$, $\gamma_{k\ell}(t)$ stands for the memory kernel and ζ_k is the stochastic force. By using averages over initial values of $q_n(0)$ and $\dot{q}_n(0)$,

$$\langle m\tilde{\omega}_n^2 q_n(0)^2 \rangle_B = m \langle \dot{q}_n(0)^2 \rangle_B = \left(\frac{\hbar\tilde{\omega}_n}{2} \right) \coth \left(\frac{\beta\hbar\tilde{\omega}_n}{2} \right), \quad (13)$$

we obtain the fluctuation-dissipation relation,

$$\frac{1}{2} \langle \zeta_k(t) \zeta_\ell(t') + \zeta_\ell(t') \zeta_k(t) \rangle_B = \sum_{n=1}^{N_B} \left(\frac{c_{kn} c_{\ell n}}{m\tilde{\omega}_n^2} \right) \left(\frac{\hbar\tilde{\omega}_n}{2} \right) \coth \left(\frac{\beta\hbar\tilde{\omega}_n}{2} \right) \cos \tilde{\omega}_n(t-t'), \quad (14)$$

$$\rightarrow k_B T \gamma_{k\ell}(t-t') \quad \text{for } \beta \rightarrow 0, \quad (15)$$

where $\langle \cdot \rangle_B$ expresses the average over initial states of the bath. $\xi_{k\ell}$ in Eq. (10) denotes a shift of oscillator frequency due to an introduced coupling, and it vanishes if we adopt

$c_n = m\tilde{\omega}_n^2$ for $N_S = 1$ [3]. In the case of $N_S \neq 1$, however, it is impossible to choose $\{c_{kn}\}$ such as $\xi_{k\ell} = 0$ for all pairs of (k, ℓ) , then Q_k is inevitably coupled with Q_ℓ ($\ell \neq k$). Because of these couplings between HOs, the N_S -body system cannot be simply regarded as a sum of systems with $N_S = 1$. Although Eqs. (9)-(12) are formally exact, it is difficult to solve N_S -coupled integrodifferential equations.

B. The canonical transformation

In order to obtain a tractable Langevin equation, we apply the canonical transformation to the model Hamiltonian. We assume that N_S is even without a loss of generality. Imposing a periodic boundary condition,

$$Q_{N_S+k} = Q_k, \quad P_{N_S+k} = P_k, \quad (16)$$

we employ the canonical transformation [20],

$$Q_k = \frac{1}{\sqrt{N_S}} \sum_{s=-N_S/2}^{N_S/2-1} e^{i(2\pi ks/N_S)} \tilde{Q}_s, \quad (17)$$

$$P_k = \frac{1}{\sqrt{N_S}} \sum_{s=-N_S/2}^{N_S/2-1} e^{i(2\pi ks/N_S)} \tilde{P}_s. \quad (18)$$

Note that the boundary condition is satisfied in Eqs. (17) and (18) and that the set $\{(1/\sqrt{N_S}) e^{i(2\pi ks/N_S)s}\}$ is orthogonal and complete in a periodic domain of the oscillator label k [20]. By the canonical transformation, H_S in Eq. (3) becomes

$$H_S = \sum_{s=-N_S/2}^{N_S/2-1} \left[\frac{\tilde{P}_s^* \tilde{P}_s}{2M} + \frac{(D + M\Omega_s^2)\tilde{Q}_s^* \tilde{Q}_s}{2} \right] - \sqrt{N_S} \tilde{Q}_0 f(t), \quad (19)$$

with

$$M\Omega_s^2 = 4K \sin^2 \left(\frac{\pi s}{N_S} \right) \quad \text{for } s = -\frac{N_S}{2}, -\frac{N_S}{2} + 1, \dots, \frac{N_S}{2} - 1, \quad (20)$$

where the commutation relations:

$$[\tilde{Q}_s, \tilde{P}_{s'}^*] = i\hbar \delta_{ss'}, \quad [\tilde{Q}_s, \tilde{Q}_{s'}] = [\tilde{P}_s, \tilde{P}_{s'}] = 0, \quad (21)$$

hold with $\tilde{Q}_s^* = \tilde{Q}_{-s}$ and $\tilde{P}_s^* = \tilde{P}_{-s}$.

For a simplicity of our calculation, we assume an identical frequency bath [14],

$$\omega_n = \omega_0, \quad c_{kn} = c. \quad (22)$$

We furthermore assume that N_B is even, imposing the periodic boundary condition given by

$$q_{N_B+n} = q_n, \quad p_{N_B+n} = p_n. \quad (23)$$

We apply the canonical transformation [14, 20],

$$q_n = \frac{1}{\sqrt{N_B}} \sum_{r=-N_B/2}^{N_B/2-1} e^{i(2\pi nr/N_B)} \tilde{q}_r, \quad (24)$$

$$p_n = \frac{1}{\sqrt{N_B}} \sum_{r=-N_B/2}^{N_B/2-1} e^{i(2\pi nr/N_B)} \tilde{p}_r, \quad (25)$$

to the bath with the periodic condition given by Eq. (23). The bath Hamiltonian H_B in Eqs. (5) becomes [25]

$$H_B = \sum_{r=-N_B/2}^{N_r/2-1} \left(\frac{\tilde{p}_r^* \tilde{p}_r}{2m} + \frac{m\omega_0^2 \tilde{q}_r^* \tilde{q}_r}{2} \right) \quad (26)$$

where the commutation relations:

$$[\tilde{q}_r, \tilde{p}_{r'}^*] = i\hbar\delta_{rr'}, \quad [\tilde{q}_r, \tilde{q}_{r'}] = [\tilde{p}_r, \tilde{p}_{r'}] = 0, \quad (27)$$

hold with $\tilde{q}_r^* = \tilde{q}_{-r}$ and $\tilde{p}_r^* = \tilde{p}_{-r}$. By canonical transformations given by Eqs. (17), (18), (24) and (25), H_I in Eq. (6) becomes

$$H_I = \frac{cN_B}{2} \sum_{s=-N_S/2}^{N_S/2-1} \tilde{Q}_s^* \tilde{Q}_s + \frac{cN_S}{2} \sum_{r=-N_B/2}^{N_B/2-1} \tilde{q}_r^* \tilde{q}_r - c\sqrt{N_S N_B} \tilde{Q}_0 \tilde{q}_0. \quad (28)$$

Summing up Eqs. (19), (26) and (28), we obtain the total Hamiltonian expressed by

$$H = H_0 + H'_S + H'_B, \quad (29)$$

where

$$H_0 = \frac{\tilde{P}_0^2}{2M} + \frac{M\tilde{\Omega}_0^2 \tilde{Q}_0^2}{2} + \frac{m\tilde{p}_0^2}{2} + \frac{m\tilde{\omega}_0^2}{2} - c\sqrt{N_S N_B} \tilde{Q}_0 \tilde{q}_0 - \sqrt{N_S} \tilde{Q}_0 f(t), \quad (30)$$

$$H'_S = \sum_{s(\neq 0)} \left[\frac{\tilde{P}_s^* \tilde{P}_s}{2M} + \frac{M\tilde{\Omega}_s^2 \tilde{Q}_s^* \tilde{Q}_s}{2} \right], \quad (31)$$

$$H'_B = \sum_{r(\neq 0)} \left[\frac{\tilde{p}_r^* \tilde{p}_r}{2m} + \frac{m\tilde{\omega}_r^2 \tilde{q}_r^* \tilde{q}_r}{2} \right], \quad (32)$$

with

$$M\tilde{\Omega}_s^2 = D + 4K \sin^2 \left(\frac{\pi s}{N_S} \right) + cN_B \quad \text{for } s = -\frac{N_S}{2}, \dots, \frac{N_S}{2} - 1, \quad (33)$$

$$m\tilde{\omega}_r^2 = m\omega_0^2 + cN_S \quad \text{for } r = -\frac{N_B}{2}, \dots, \frac{N_B}{2} - 1. \quad (34)$$

It is noted that H_0 expresses the Hamiltonian for a uniform mode with $s = u = 0$ and that a summation over s (r) in the H'_S (H'_B) is excluded for $s = 0$ ($r = 0$).

C. Eigenfrequencies with $f(t) = 0$

Eigenfrequencies of the system-plus-bath with $f(t) = 0$ may be obtained when we diagonalize H_0 given by Eq. (30). We employ the canonical transformation given by

$$\tilde{Q}_0 = M^{-1/2}(X_1 \cos \theta + X_2 \sin \theta), \quad \tilde{P}_0 = M^{1/2}(Y_1 \cos \theta + Y_2 \sin \theta), \quad (35)$$

$$\tilde{q}_0 = m^{-1/2}(-X_1 \sin \theta + X_2 \cos \theta), \quad \tilde{p}_0 = m^{1/2}(-Y_1 \sin \theta + Y_2 \cos \theta), \quad (36)$$

where $Y_i = \dot{X}_i$ and their commutation relations are given by

$$[X_i, Y_j] = i\hbar\delta_{ij}, \quad [X_i, X_j] = [Y_i, Y_j] = 0 \quad \text{for } i, j = 1, 2. \quad (37)$$

The canonical transformation yields the diagonalized Hamiltonian given by

$$H = H_0 + H'_S + H'_B, \quad (38)$$

with

$$H_0 = \frac{Y_1^2}{2} + \frac{\phi_1^2 X_1^2}{2} + \frac{Y_2^2}{2} + \frac{\phi_2^2 X_1^2}{2}, \quad (39)$$

$$\tan 2\theta = \frac{2c\sqrt{N_S N_B}}{\sqrt{Mm}(\tilde{\Omega}_0^2 - \tilde{\omega}_0^2)}, \quad (40)$$

$$\phi_1^2 = \tilde{\Omega}_0^2 \cos^2 \theta + \tilde{\omega}_0^2 \sin^2 \theta + \left(\frac{2c\sqrt{N_S N_B}}{\sqrt{Mm}} \right) \cos \theta \sin \theta, \quad (41)$$

$$\phi_2^2 = \tilde{\Omega}_0^2 \sin^2 \theta + \tilde{\omega}_0^2 \cos^2 \theta - \left(\frac{2c\sqrt{N_S N_B}}{\sqrt{Mm}} \right) \cos \theta \sin \theta, \quad (42)$$

where H'_S and H'_B are given by Eqs. (31) and (32), respectively. With the use of Eq. (40), ϕ_1^2 and ϕ_2^2 are alternatively expressed by

$$\phi_{1,2}^2 = \frac{1}{2} \left[\tilde{\Omega}_0^2 + \tilde{\omega}_0^2 \pm \sqrt{(\tilde{\Omega}_0^2 - \tilde{\omega}_0^2)^2 + \frac{4N_S N_B c^2}{Mm}} \right], \quad (43)$$

where + (−) of a double sign is applied to ϕ_1^2 (ϕ_2^2).

In the equilibrium state with $f(t) = 0$, Eqs. (31), (32) and (43) yield eigenfrequencies of $\{\nu_i\}$ ($i = 1$ to $N_S + N_B$) for H given by

i	1	...	$N_S/2 + 1$...	N_S	$N_S + 1$...	$N_S + N_B/2 + 1$...	$N_S + N_B$
ν_i^2	$\tilde{\Omega}_{-N_S/2}^2$...	ϕ_1^2	...	$\tilde{\Omega}_{N_S/2-1}^2$	$\tilde{\omega}_0^2$...	ϕ_2^2	...	$\tilde{\omega}_0^2$

In the limit of $c = 0$, eigenfrequencies become

i	1	...	$N_S/2 + 1$...	N_S	$N_S + 1$...	$N_S + N_B/2 + 1$...	$N_S + N_B$
ν_i^2	$\Omega_{-N_S/2}^2$...	Ω_0^2	...	$\Omega_{N_S/2-1}^2$	ω_0^2	...	ω_0^2	...	ω_0^2

Reference [14] obtained the same eigenfrequencies by an alternative method: ϕ_1 and ϕ_2 given by Eq. (43) correspond to ν_+ and ν_- , respectively, in Ref. [14]. With the use of these eigenfrequencies, the system energy E_S is given by [14]

$$E_S = -\frac{\partial \ln Z_S}{\partial \beta}, \quad (44)$$

$$= \sum_{i=1}^{N_S+N_B} \left(\frac{\hbar\nu_i}{2} \right) \coth \left(\frac{\beta\hbar\nu_i}{2} \right) - \left(\frac{N_B\hbar\omega_0}{2} \right) \coth \left(\frac{\beta\hbar\omega_0}{2} \right), \quad (45)$$

where

$$Z_S = \frac{Z}{Z_B}, \quad (46)$$

with

$$Z = \text{Tr } e^{-\beta H} = \prod_{i=1}^{N_S+N_B} \left[\frac{1}{2 \sinh(\beta\hbar\nu_i/2)} \right], \quad (47)$$

$$Z_B = \text{Tr}_B e^{-\beta H_B} = \left[\frac{1}{2 \sinh(\beta\hbar\omega_0/2)} \right]^{N_B}, \quad (48)$$

Tr and Tr_B denoting a full trace over all variables and a partial trace over bath variables, respectively.

D. Responses to external forces

1. Driven quantum harmonic oscillators

Quantum HOs driven by an external force have been discussed in Refs. [21–23]. It has been shown that the average position of a quantum HO is expressed by an equation of

motion of relevant classical HO [21–23] as follows. The Hamiltonian of a single HO with mass m and oscillating frequency ω_0 driven by a force $F(t)$ is given by [21–23]

$$H = \frac{p^2}{2m} + \frac{m\omega_0^2 x^2}{2} - xF(t), \quad (49)$$

for which the Schrödinger equation is expressed by

$$\left[-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{m\omega_0^2 x^2}{2} - xF(t) \right] \Phi(x, t) = i\hbar \frac{\partial \Phi(x, t)}{\partial t}. \quad (50)$$

By using a unitary transformation, we may obtain a solution of $\Phi(x, t)$ expressed by [24]

$$\Phi_n(x, t) = \phi_n(x - w(t)) \exp \left\{ \frac{i}{\hbar} \left[m\dot{w}(x - w(t)) - E_n t + \int_0^t L(t') dt' \right] \right\}, \quad (51)$$

with

$$L(t) = \frac{1}{2}m\ddot{w}^2 - \frac{1}{2}m\omega_0^2 w^2 + wF(t), \quad (52)$$

$$E_n = \hbar\omega_0 \left(n + \frac{1}{2} \right) \quad \text{for } n = 0, 1, 2, \dots. \quad (53)$$

Here $\phi_n(x)$ and E_n are wavefunction and eigenvalue, respectively, of the Schrödinger equation with $F(t) = 0$ in Eq. (49), and $w(t)$ obeys an equation of motion for a classical driven HO,

$$m\ddot{w}(t) + m\omega_0^2 w(t) = F(t). \quad (54)$$

Equation (51) shows that the center of a wave packet moves with $w(t)$. It implies that an average of time-dependent position is given by [21–23]

$$\overline{x}(t) = w(t), \quad (55)$$

where an overline denotes the quantum average and $w(t)$ is a solution of Eq. (54). This is consistent with Ehrenfest's theorem.

2. Open quantum system of harmonic oscillators

In order to study the response of the open quantum HO under consideration, it is necessary to pursue equations of classical motions after Husimi's method [21–23]. From Eqs. (30) and (35), the total Hamiltonian with $f(t) \neq 0$ becomes

$$H = H_0 + H'_S + H'_B, \quad (56)$$

with

$$H_0 = H_{01} + H_{02}, \quad (57)$$

$$H_{01} = \frac{Y_1^2}{2} + \frac{\phi_1^2 X_1^2}{2} - \sqrt{\frac{N_S}{M}} X_1 f(t) \cos \theta, \quad (58)$$

$$H_{02} = \frac{Y_2^2}{2} + \frac{\phi_2^2 X_2^2}{2} - \sqrt{\frac{N_S}{M}} X_2 f(t) \sin \theta, \quad (59)$$

where H'_S and H'_B are given by Eqs. (31) and (32), respectively, and ϕ_1 and ϕ_2 are given by Eqs. (41) and (42). Hamiltonians H_{01} and H_{02} in Eqs. (58) and (59) express HOs driven by forces of $\sqrt{N_S/M} f(t) \cos \theta$ and $\sqrt{N_S/M} f(t) \sin \theta$, respectively. From H'_S in Eq. (31), equations of motion for \tilde{Q}_s with $s \neq 0$ are given by

$$M\ddot{\tilde{Q}}_s = -M\tilde{\Omega}_s^2 \tilde{Q}_s \quad \text{for } s \neq 0, \quad (60)$$

while Eqs. (57) and (58) lead to those for $s = 0$, X_1 and X_2 , given by

$$\ddot{X}_1 = -\phi_1^2 X_1 + \sqrt{\frac{N_S}{M}} f(t) \cos \theta, \quad (61)$$

$$\ddot{X}_2 = -\phi_2^2 X_2 + \sqrt{\frac{N_S}{M}} f(t) \sin \theta. \quad (62)$$

A solution for $\tilde{Q}_0(t)$ may be evaluated from solutions of $X_1(t)$ and $X_2(t)$ with the canonical transformation given by Eq. (35).

After some manipulations, quantum-averaged solutions of \tilde{Q}_s are given by

$$\bar{\tilde{Q}}_s(t) = \tilde{Q}_s(0) \cos \tilde{\Omega}_s t + \frac{\tilde{P}_s(0)}{M\tilde{\Omega}_s} \sin \tilde{\Omega}_s t \quad \text{for } s \neq 0, \quad (63)$$

$$\bar{\tilde{Q}}_0(t) = \tilde{Q}_0(0) A_Q(t) + \tilde{P}_0(0) A_P(t) + \tilde{q}_0(0) B_q(t) + \tilde{p}_0(0) B_p(t) + \Phi(t) \quad \text{for } s = 0, \quad (64)$$

with

$$A_Q(t) = \sum_{i=1}^2 a_i \cos \phi_i t, \quad (65)$$

$$A_P(t) = \frac{1}{M} \sum_{i=1}^2 \frac{a_i \sin \phi_i t}{\phi_i}, \quad (66)$$

$$B_q(t) = -\sqrt{\frac{m}{M}} \cos \theta \sin \theta (\cos \phi_1 t - \cos \phi_2 t), \quad (67)$$

$$B_p(t) = -\frac{1}{\sqrt{Mm}} \cos \theta \sin \theta \left(\frac{\sin \phi_1 t}{\phi_1} - \frac{\sin \phi_2 t}{\phi_2} \right), \quad (68)$$

$$\Phi(t) = \frac{\sqrt{N_S}}{M} \sum_{i=1}^2 \left(\frac{a_i}{\phi_i} \right) \int_0^t \sin \phi_i(t-t') f(t') dt', \quad (69)$$

$$a_1 = 1 - a_2 = \cos^2 \theta, \quad (70)$$

where $\tilde{Q}_s(0)$, $\tilde{P}_s(0)$, $\tilde{q}_s(0)$ and $\tilde{p}_s(0)$ denote initial states. The response of the total output averaged over initial states is given by

$$R(t) \equiv \left\langle \sum_k \overline{Q}_k(t) \right\rangle_0 = \sqrt{N_S} \left\langle \overline{\tilde{Q}}_0(t) \right\rangle_0, \quad (71)$$

$$= \frac{N_S}{M} \sum_{i=1}^2 \left(\frac{a_i}{\phi_i} \right) \int_0^t \sin \phi_i(t-t') f(t') dt', \quad (72)$$

where we employ the relations given by

$$\left\langle \tilde{Q}_s(0) \right\rangle_0 = \left\langle \tilde{P}_s(0) \right\rangle_0 = \langle \tilde{q}_s(0) \rangle_0 = \langle \tilde{p}_s(0) \rangle_0 = 0, \quad (73)$$

the bracket $\langle \cdot \rangle_0$ expressing an average over initial states. Equation (72) leads to the susceptibility,

$$\chi(t) = \frac{N_S}{M} \sum_{i=1}^2 \frac{a_i \sin \phi_i t}{\phi_i}, \quad (74)$$

whose Fourier transformation is given by

$$\hat{\chi}(\omega) = \frac{N_S}{M} \sum_{i=1}^2 \frac{a_i}{(\phi_i^2 - \omega^2)}, \quad (75)$$

with poles at $\omega = \pm \phi_i$.

It should be noted that $R(t)$ in Eq. (72) is generally not proportional to N_S except for the $c = 0$ case because ϕ_i and a_i depend on N_S as shown in Eqs. (41), (42) and (70). This point will be shortly demonstrated in numerical model calculations for sinusoidal and step forces in the following.

A. Sinusoidal forces

We apply a periodic monochromatic force,

$$f(t) = g \sin \omega t, \quad (76)$$

where ω and g stand for the frequency and magnitude, respectively, of the force. Equations (72) and (76) yield

$$R(t) = \left(\frac{N_S g}{M} \right) \sum_{i=1}^2 \frac{a_i (\phi_i \sin \omega t - \omega \sin \phi_i t)}{\phi_i (\phi_i^2 - \omega^2)} \quad \text{for } \omega \neq \phi_i. \quad (77)$$

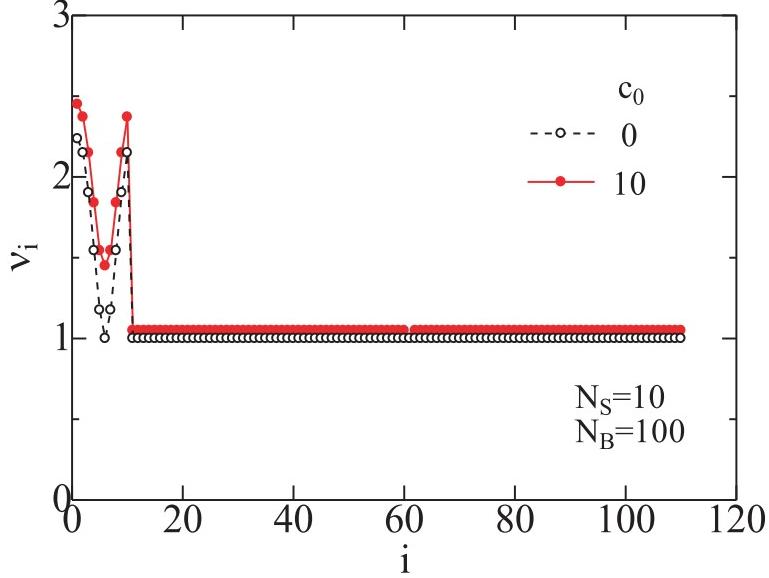


FIG. 1: (Color online) Eigenfrequencies ν_i of HO systems with $N_S = 10$ subjected to a bath with $N_B = 100$ for $c_0 = 0.0$ (open circles) and $c_0 = 10.0$ (filled circles) ($D = K = M = m = 1.0$ and $\omega_0 = 1.0$), solid and dashed curves being plotted only for a guide of the eye.

In the resonant case of $\omega = \phi_1$, $R(t)$ is given by

$$R(t) = \left(\frac{N_S g}{M} \right) \left[\frac{a_1 (\sin \omega t - \omega t \cos \omega t)}{2\omega^2} + \frac{a_2 (\phi_2 \sin \omega t - \omega \sin \phi_2 t)}{\phi_2(\phi_2^2 - \omega^2)} \right]. \quad (78)$$

Expressions of $R(t)$ in the resonance cases of $\omega = \phi_2$ and $\omega = \phi_1 = \phi_2$ are similarly given. In the limit of $c = 0$ where $\phi_1 = \Omega_0$, $\phi_2 = \omega_0$, $\theta = 0.0$, $a_1 = 1.0$ and $a_2 = 0.0$, Eq. (77) reduces to

$$R(t) = \left(\frac{N_S g}{M} \right) \left[\frac{\Omega_0 \sin \omega t - \omega \sin \Omega_0 t}{\Omega_s(\Omega_0^2 - \omega^2)} \right] \quad \text{for } c = 0 \text{ and } \omega \neq \Omega_0, \quad (79)$$

which expresses the response of a HO isolated from a bath.

We have performed numerical model calculations, choosing a coupling [14],

$$c = \frac{c_0}{N_S N_B}, \quad (80)$$

such that the interaction term in Eq. (6) including summations over $\sum_{k=1}^{N_S}$ and $\sum_{n=1}^{N_B}$ yield finite contributions even in the limits of $N_S \rightarrow \infty$ and/or $N_B \rightarrow \infty$. We have adopted parameters of $D = K = M = m = \omega_0 = 1.0$ for a given system-plus-bath.

Figure 1 shows eigenfrequencies ν_i for $c_0 = 0.0$ (open circles) and $c_0 = 10.0$ (filled circles) of a HO system ($N_S = 10$) subjected to a bath ($N_B = 100$). Eigenfrequencies ν_i for

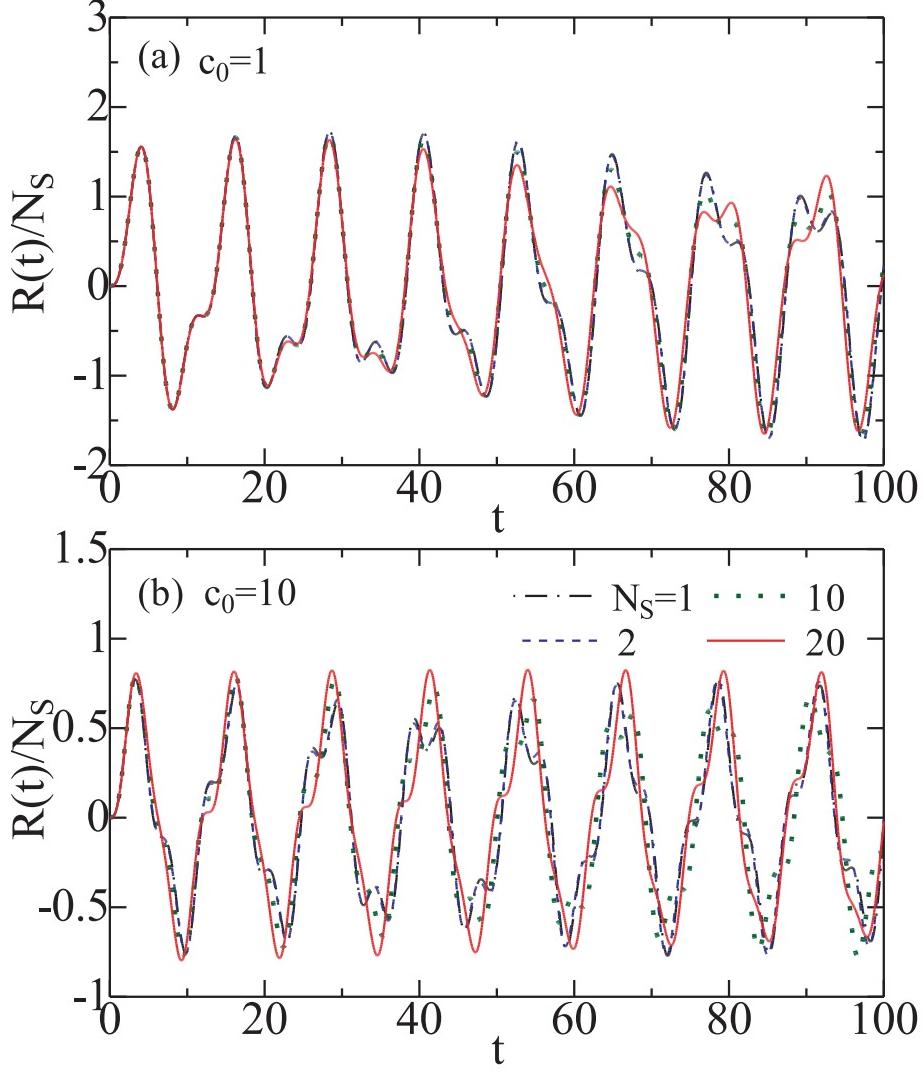


FIG. 2: (Color online) Responses of $R(t)/N_S$ of HO systems with $N_S = 1$ (chain curves), 2 (dashed curves), 10 (dotted curves) and 20 (solid curves) for (a) $c_0 = 1.0$ and (b) $c_0 = 10.0$ to an applied sinusoidal force with $\omega = 0.5$ and $g = 1.0$ ($D = K = M = m = 1.0$, $\omega_0 = 1.0$ and $N_B = 100$).

$1 \leq i \leq 10$ show a dispersion relation of the HO system while those for $11 \leq \nu_i \leq 110$ of the bath are almost constant. For $c_0 = 0.0$, we obtain $\tilde{\Omega}_0 = 1.0$ and $\tilde{\omega}_0 = 1.0$. When the system-bath coupling of $c_0 = 10.0$ is introduced, they become 1.414 and 1.048, respectively, which lead to $\phi_1 = 1.449$ and $\phi_2 = 1.0$.

Figure 2(a) shows responses of $R(t)/N_S$ to a sinusoidal force with $\omega = 0.5$ and $g = 1.0$ of HO systems with $N_S = 1, 2, 10$ and 20 coupled to $N_B = 100$ baths with a coupling

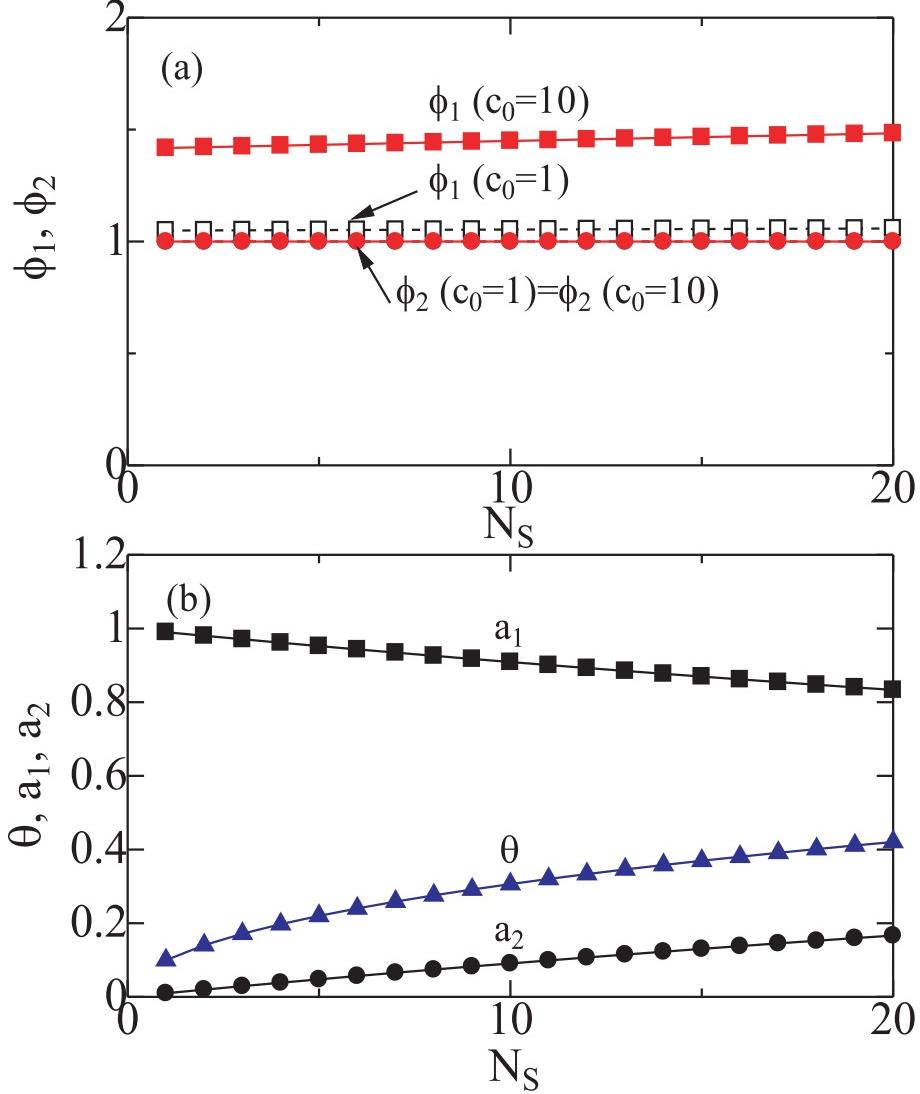


FIG. 3: (Color online) N_S dependences of (a) ϕ_i , and (b) θ and a_i ($i = 1, 2$) for $c_0 = 1.0$ (dashed curves) and 10.0 (solid curves) ($D = K = M = m = \omega_0 = 1.0$ and $N_B = 100$). θ and a_i in (b) are independent of c_0 for the adopted parameters (see the text).

of $c_0 = 1.0$. Results of $R(t)/N_S$ are almost the same independently of N_S , although some discrepancies among the four results are realized at $t \gtrsim 50$. These discrepancies become more evident for a larger coupling of $c_0 = 10.0$, whose results are shown in Fig. 2(b). These results clearly suggest

$$R(t; N_S) = N_S R(t; 1) \quad \text{for } c = 0, \quad (81)$$

$$\neq N_S R(t; 1) \quad \text{for } c \neq 0. \quad (82)$$

In order to elucidate N_S and c_0 dependences of $R(t)/N_S$, we show in Figs. 3, ϕ_i , θ and a_i ($i = 1, 2$) as a function of N_S for $c_0 = 1.0$ (dashed curves) and 10.0 (solid curves). Figure 3(a) shows that with increasing N_S , ϕ_1 is slightly increased while ϕ_2 is constant. We note in Fig. 3(b) that an increase of N_S yields an increase in θ , by which a_2 is increased but a_1 is decreased. For adopted parameters, θ , a_1 and a_2 are independent of c because the denominator of Eq. (40) becomes $\tilde{\Omega}_0^2 - \tilde{\omega}_0^2 = (N_B - N_S)c$ whose c is cancelled out by that in its numerator. With increasing N_S , a contribution from a lower eigenfrequency of ϕ_2 is increased. The effect of the system-bath coupling for $c_0 = 10.0$ is more significant than that for $c_0 = 1.0$ because the difference of $\phi_1 - \phi_2$ in the former is larger than that in the latter: if $\phi_1 = \phi_2$ results are independent of a_i (and then N_S).

B. Step forces

Next we apply a step force given by

$$f(t) = g \Theta(t_s - t), \quad (83)$$

where $\Theta(x)$ stands for the Heaviside function and t_s is the starting time of a force with a magnitude of g . The averaged output is given by

$$R(t) = \left(\frac{N_S g}{M} \right) \sum_{i=1}^2 \frac{a_i [1 - \cos \phi_i(t - t_s)]}{\phi_i^2}. \quad (84)$$

Figure 4(a) shows $R(t)/N_S$ for a step force with $t_s = 10.0$ and $g = 1.0$ of HO systems with $N_S = 1, 2, 10$ and 20 coupled to $N_B = 100$ baths with a coupling of $c_0 = 1.0$ ($D = 1.0$ and $\omega_0 = 1.0$). Result of $R(t)/N_S$ for $N_S \geq 2$ are almost the same as that for $N_S = 1$. However, when the interaction is increased to $c_0 = 10.0$, the discrepancy between results of $N_S = 1$ and $N_S \geq 2$ become evident. Fig. 4(b) shows similar plots but with stronger coupling of $c_0 = 10.0$, for which shape and magnitude of $R(t)/N_S$ are significantly modified for $N_S \geq 2$.

III. DISCUSSION

A. Responses to space- and time-dependent forces

It is interesting to calculate responses to a space- and time-dependent force which yields H_f in Eq. (3),

$$H_f = -f(t)S(u), \quad (85)$$

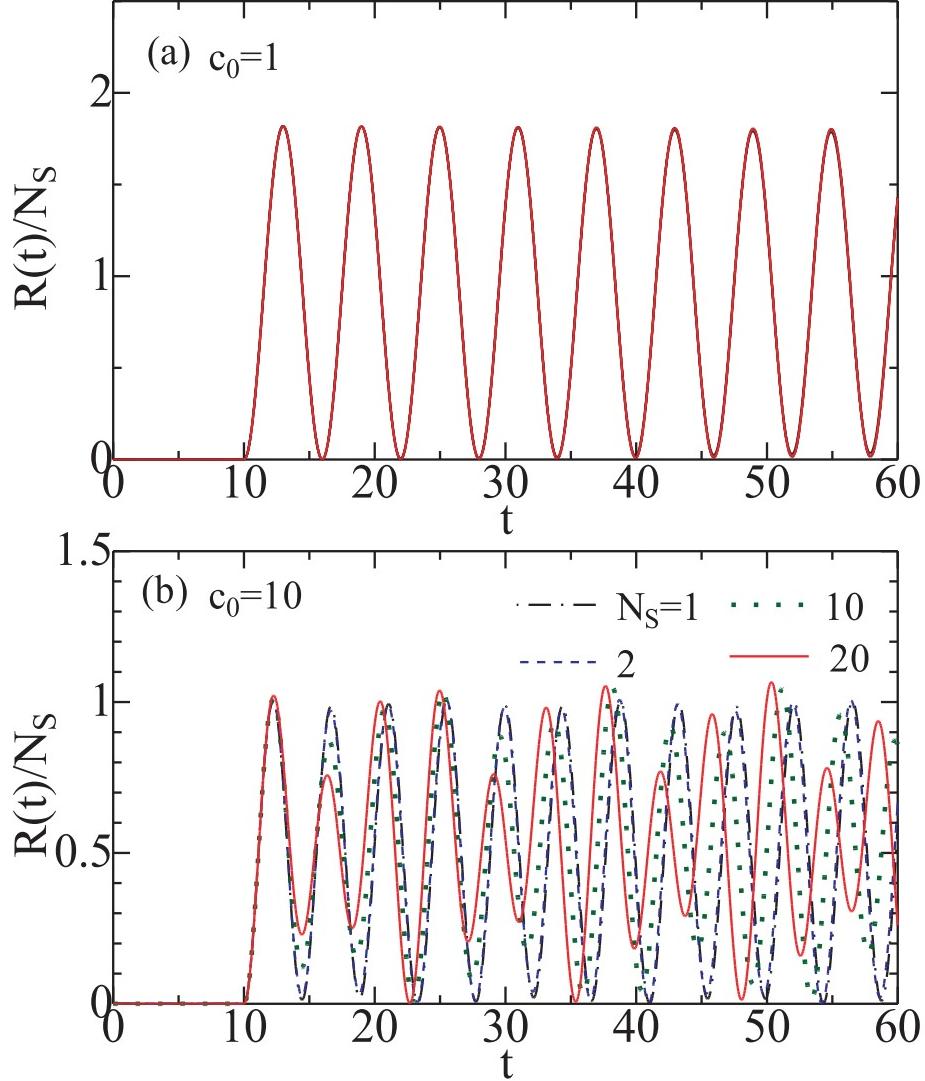


FIG. 4: (Color online) Responses of $R(t)/N_S$ of HO systems with $N_S = 1$ (chain curves), 2 (dashed curves), 10 (dotted curves) and 20 (solid curves) for (a) $c_0 = 1.0$ and (b) $c_0 = 10.0$ to an applied step force with $t_s = 10.0$ and $g = 1.0$ ($B = K = M = m = 1.0$, $\omega_0 = 1.0$ and $N_B = 100$). Results for all N_S in (a) are indistinguishable.

with

$$S(u) = \sum_{k=1}^{N_B} Q_k e^{i2\pi k u / N_S} \quad \text{for } u \in \left\{-\frac{N_S}{2}, -\frac{N_S}{2} + 1, \dots, \frac{N_S}{2} - 1\right\}. \quad (86)$$

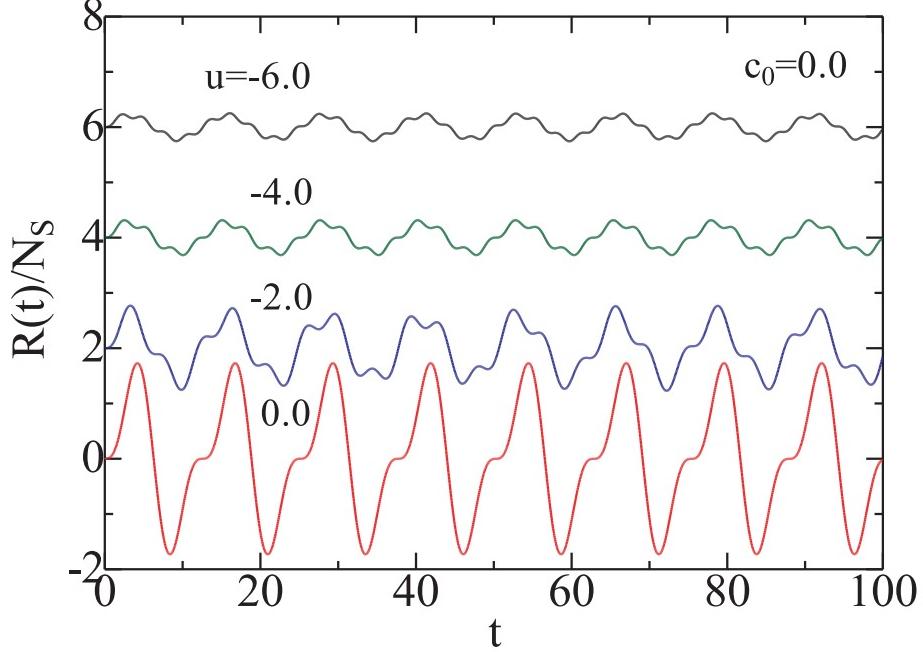


FIG. 5: (Color online) Responses of $R(t)/N_S$ of an isolated HO system ($c_0 = 0.0$) to an applied sinusoidal force with $\omega = 0.5$ and $g = 1.0$ for various u ($N_S = 12$, $N_B = 100$ and $K = D = M = m = \omega_0 = 1.0$). Results for $u = -6.0$, -4.0 and -2.0 are shifted by 6.0, 4.0 and 2.0, respectively, for clarity of the figures.

Here the wavevector u is, for example, $u = 0$ and $u = -N_S/2$ for uniform and staggered forces, respectively, for which $S(u)$ is represented by

$$S(u) = \sum_{k=1}^{N_S} Q_k \quad \text{for } u = 0, \quad (87)$$

$$= \sum_{k=1}^{N_S} Q_k e^{-i\pi k} \quad \text{for } u = -\frac{N_S}{2}. \quad (88)$$

The mode with $u \neq 0$ does not couple with $s = 0$ mode which couples with bath as mentioned in the preceding subsection II D. Equations of motion for \tilde{Q}_s with $s \neq 0$ are independent of degrees of freedom in a bath and they are given by

$$M\ddot{\tilde{Q}}_u = -M\tilde{\Omega}_u^2\tilde{Q}_u + \sqrt{N_S}f(t) \quad \text{for } s \neq 0 \text{ and } s = u \neq 0, \quad (89)$$

$$M\ddot{\tilde{Q}}_s = -M\tilde{\Omega}_s^2\tilde{Q}_s \quad \text{for } s \neq 0 \text{ and } s \neq u \neq 0. \quad (90)$$

The response to applied force with $u (\neq 0)$ is given by

$$R(t) = \left(\frac{N_S g}{M} \right) \int_0^t \frac{\sin \tilde{\Omega}_u(t-t')f(t')}{\tilde{\Omega}_u} dt', \quad (91)$$

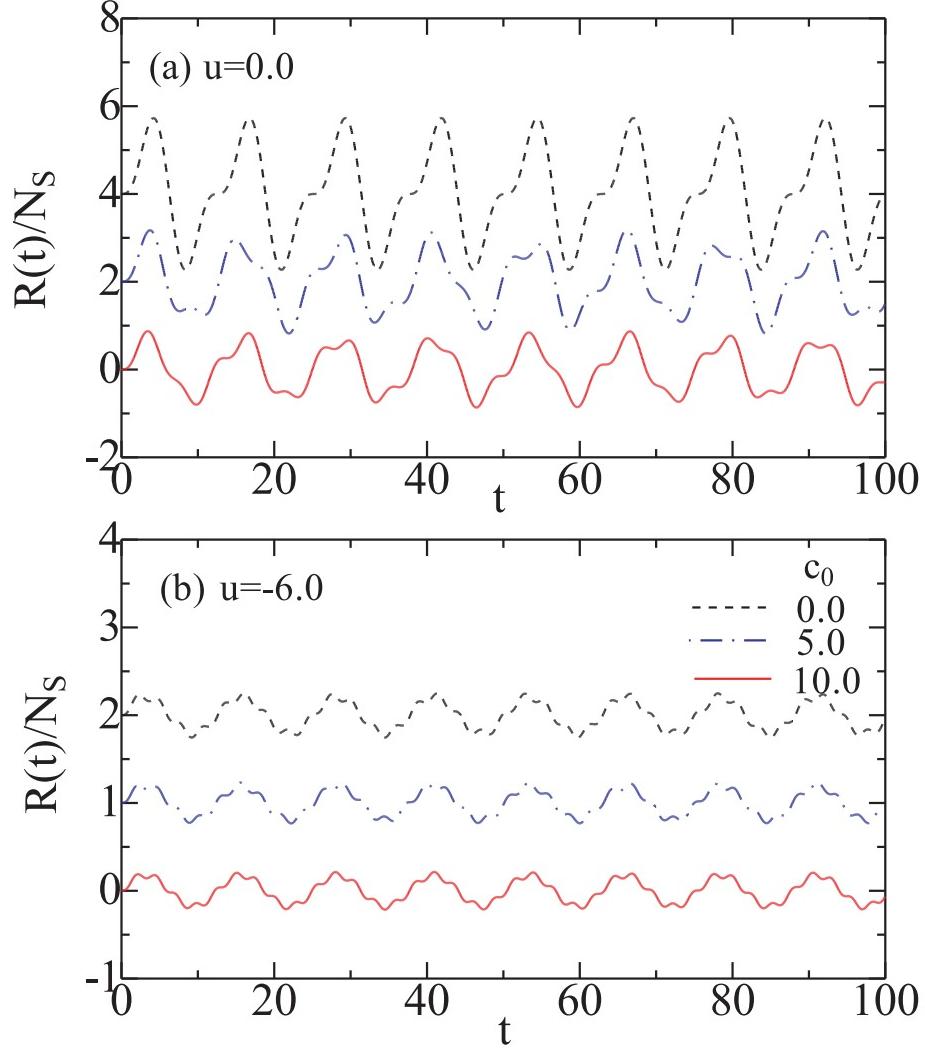


FIG. 6: (Color online) Responses of $R(t)/N_S$ of HO systems coupled with $c_0 = 0.0$ (dashed curves), $c_0 = 5.0$ (chain curves) and $c_0 = 10.0$ (solid curves) to an applied sinusoidal force with $\omega = 0.5$ and $g = 1.0$ for (a) $u = 0.0$ and (b) $u = -6.0$ ($N_S = 12$, $N_B = 100$ and $K = B = M = m = \omega_0 = 1.0$). Results for $c_0 = 0.0, 5.0$ in (a) are shifted by 4.0 and 2.0, respectively, and those for $c_0 = 0.0, 5.0$ in (b) are similarly shifted by 2.0 and 1.0, for clarity of the figures.

which becomes for sinusoidal force [Eq. (76)],

$$R(t) = \left(\frac{N_S g}{M} \right) \left(\frac{\tilde{\Omega}_u \sin \omega t - \omega \sin \tilde{\Omega}_u t}{\tilde{\Omega}_u (\tilde{\Omega}_u^2 - \omega^2)} \right). \quad (92)$$

In the limit of $c = 0.0$, $R(t)$ is given by Eqs. (91) and (92) with $\tilde{\Omega}_u = \Omega_u$. The effect of finite coupling is realized by a change in $\tilde{\Omega}_u$ as given by Eq. (33). Note that the response to applied force with $u = 0$ has been studied in subsection II D [Eq. (72)].

We present model calculations for sinusoidal forces with $\omega = 0.5$ and $g = 1.0$ in Eq. (76) for $N_S = 12$, $N_B = 100$, $K = B = M = m = \omega_0 = 1.0$. Figure 5 shows $R(t)/N_S$ for isolated systems ($c_0 = 0.0$) with $u = 0.0, -2.0, -4.0$ and -6.0 . Magnitudes of $R(t)/N_S$ become smaller for larger $|u|$. Figure 6(a) and 6(b) show $R(t)/N_S$ for uniform ($u = 0.0$) and staggered forces ($u = -6.0$), respectively, with couplings of $c_0 = 0.0$ (dashed curve), 5.0 (chain curve) and 10.0 (solid curve). Comparing Fig. 6(b) with Fig. 6(a), we notice that an effect of couplings for staggered forces is less effective than that for uniform forces.

B. Spatial correlation

Employing eigenfrequencies for $f(t) = 0$ obtained in subsection II C, we may calculate the spatial correlation between Q_k and Q_{k+m} ,

$$\Gamma_m \equiv \sum_{k=1}^{N_S} \langle Q_k Q_{k+m} \rangle, \quad (93)$$

$$= \sum_{s=-N_S/2}^{N_S/2-1} \langle \tilde{Q}_s^* \tilde{Q}_s \rangle e^{-i 2\pi ms/N_S}, \quad (94)$$

with $\langle \tilde{Q}_s^* \tilde{Q}_s \rangle$ evaluated by [19]

$$\langle \tilde{Q}_s^* \tilde{Q}_s \rangle = - \left(\frac{1}{\beta M \tilde{\Omega}_s} \right) \frac{\partial \ln Z_S}{\partial \tilde{\Omega}_s}, \quad (95)$$

where the bracket $\langle \rangle$ denotes the average over H and Z_S is given by Eq. (46). Γ_m with $m = 0$ expresses a (summed) variance of Q_k : $\Gamma_0 = \sum_{k=1}^{N_S} \langle Q_k^2 \rangle$. After some manipulations with the use of the diagonalized Hamiltonian given by Eq. (38), we obtain

$$\langle \tilde{Q}_s^* \tilde{Q}_s \rangle = \frac{\hbar}{2M\tilde{\Omega}_s} \coth \left(\frac{\beta \hbar \tilde{\Omega}_s}{2} \right) \quad \text{for } s \neq 0, \quad (96)$$

$$= \frac{\hbar}{2M\tilde{\Omega}_0} \sum_{i=1}^2 \coth \left(\frac{\beta \hbar \phi_i}{2} \right) \left(\frac{\partial \phi_i}{\partial \tilde{\Omega}_0} \right) \quad \text{for } s = 0, \quad (97)$$

with

$$\frac{\partial \phi_1}{\partial \tilde{\Omega}_0} = \frac{\tilde{\Omega}_0}{2\phi_1} \left[1 + \frac{\tilde{\Omega}_0^2 - \omega_0^2}{\sqrt{(\tilde{\Omega}_0^2 - \omega_0^2)^2 + 4N_S N_B c^2 / Mm}} \right], \quad (98)$$

$$\frac{\partial \phi_2}{\partial \tilde{\Omega}_0} = \frac{\tilde{\Omega}_0}{2\phi_2} \left[1 - \frac{\tilde{\Omega}_0^2 - \omega_0^2}{\sqrt{(\tilde{\Omega}_0^2 - \omega_0^2)^2 + 4N_S N_B c^2 / Mm}} \right], \quad (99)$$

where ϕ_1 and ϕ_2 are given by Eqs. (40) and (41). Substituting Eqs. (96) and (97) into Eq. (??), we obtain Γ_m ,

$$\begin{aligned}\Gamma_m = & \sum_{s=-N_S/2}^{N_S/2-1} \frac{\hbar}{2M\tilde{\Omega}_s} \coth\left(\frac{\beta\hbar\tilde{\Omega}_s}{2}\right) e^{-i2\pi ms/N_s} \\ & + \frac{\hbar}{2M\tilde{\Omega}_0} \left[\sum_{i=1}^2 \coth\left(\frac{\beta\hbar\phi_i}{2}\right) \left(\frac{\partial\phi_i}{\partial\tilde{\Omega}_0} \right) - \coth\left(\frac{\beta\hbar\tilde{\Omega}_0}{2}\right) \right].\end{aligned}\quad (100)$$

For $T = 0$ and $T \rightarrow \infty$, Γ_m becomes

$$\Gamma_m = \sum_{s=-N_S/2}^{N_S/2-1} \left(\frac{\hbar}{2M\tilde{\Omega}_s} \right) e^{-i2\pi ms/N_s} + \frac{\hbar}{2M\tilde{\Omega}_0} \left[\sum_{i=1}^2 \left(\frac{\partial\phi_i}{\partial\tilde{\Omega}_0} \right) - 1 \right] \quad \text{for } T = 0, \quad (101)$$

$$= \sum_{s=-N_S/2}^{N_S/2-1} \left(\frac{k_B T}{M\tilde{\Omega}_s^2} \right) e^{-i2\pi ms/N_s} + \frac{k_B T}{M\tilde{\Omega}_0} \left[\sum_{i=1}^2 \frac{\partial \ln \phi_i}{\partial \tilde{\Omega}_0} - \frac{1}{\tilde{\Omega}_0} \right] \quad \text{for } T \rightarrow \infty. \quad (102)$$

In the case of uncoupled, isolated system with $K = 0.0$ and $c = 0.0$, Γ_m is given by

$$\Gamma_m = \delta_{m0} \left(\frac{N_S \hbar}{2M\tilde{\Omega}_0} \right) \coth\left(\frac{\beta\hbar\tilde{\Omega}_0}{2}\right) \quad \text{for } K = 0.0 \text{ and } c_0 = 0.0, \quad (103)$$

which is proportional to N_S and which vanishes for $m \geq 1$. It is, however, not the case for $K \neq 0.0$ or $c \neq 0.0$. Indeed in the case of $K \neq 0.0$, Γ_m is finite for $m \geq 1$ because of direct particle-particle couplings of K and indirect couplings of $-c_{k\ell}c_{\ell n}/m\tilde{\omega}_n^2$ in the second term of Eq. (10). Even when $K = 0.0$, Γ_m with $c \neq 0.0$ remains finite with a small negative value.

Figure 7 shows the temperature dependence of $\Gamma_m(T)/N_S$ for $m = 0$ (solid curve), 1 (dashed curve) and 2 (chain curve) of HO systems with $N_S = 10$, $N_B = 100$, $K = D = M = m = \omega_0 = 1.0$ and $c_0 = 10.0$. $\Gamma_m(T)$ is finite at $T = 0$, and at $T \rightarrow \infty$ it is proportional to temperature, as Eqs. (101) and (102) show. Magnitude of Γ_m is smaller for a larger m . The dotted curve expresses C_0 ($= \langle \tilde{Q}_0^* \tilde{Q}_0 \rangle$) which is larger than Γ_0 because $\tilde{\Omega}_0 < \tilde{\Omega}_s$ with $s \neq 0$.

N_S dependences of $\Gamma_0(T)/N_S$ at $k_B T / \hbar\omega_0 = 0.0$ and 10.0 are shown in Fig. 8(a) and 8(b), respectively, for $c_0 = 0.0$ (open circles), 1.0 (filled square) and 10.0 (filled circles). For $c_0 = 0.0$, $\Gamma_0(0)$ is proportional to N_S as expected. However, when the system-bath coupling is introduced, Γ_0 is not proportional to N_S as shown in Fig. 8. This is realized not only at zero temperature but also at high temperature.

Even when external forces are applied, the spatial correlation is not modified, which is the characteristics of the open system with the linear system-bath coupling. In the open system with the nonlinear system-bath coupling, the spatial correlation is modified by an applied force [26].

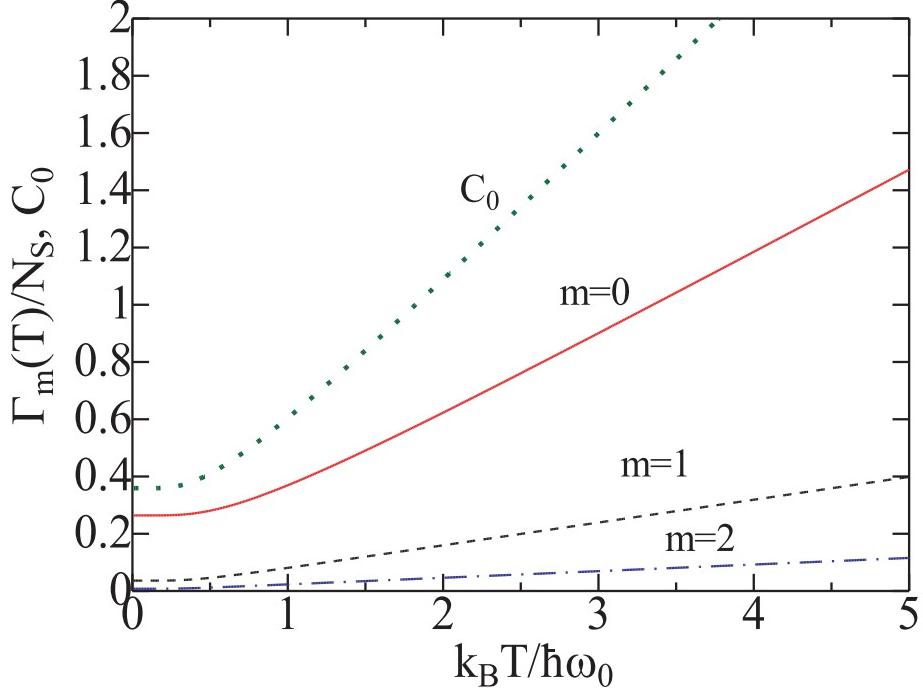


FIG. 7: (Color online) The temperature dependence of $\Gamma_m(T)/N_S$ for $m = 0$ (solid curve), $m = 1$ (dashed curve), $m = 2$ (chain curve) and C_0 ($= \langle \tilde{Q}_0^* \tilde{Q}_0 \rangle$) (dotted curve) for a HO system ($N_S = 10$, $N_B = 100$, $K = D = M = m = \omega_0 = 1.0$ and $c_0 = 10.0$)

IV. CONCLUSION

Responses of open small quantum systems described by the $(N_S + N_B)$ model [13, 14] have been studied. By using double canonical transformations mentioned in subsections II B and II C, we obtain the diagonalized Hamiltonian, from which the response to applied forces is obtained with the use of Husimi's method for a driven quantum HO [21]. The response to a uniform force given by Eq. (4) is generally not proportional to N_S against our implicit expectation. This nonlinear response is consistent with the system specific heat in open small quantum systems previously discussed in Ref. [14], and it is realized also in spatial correlation Γ_m not only at low temperatures but also at high temperatures. These facts show an importance of taking account of finite N_S in discussing open quantum and classical systems. It would be interesting to examine the obtained non-linearly by experiments for open small systems.

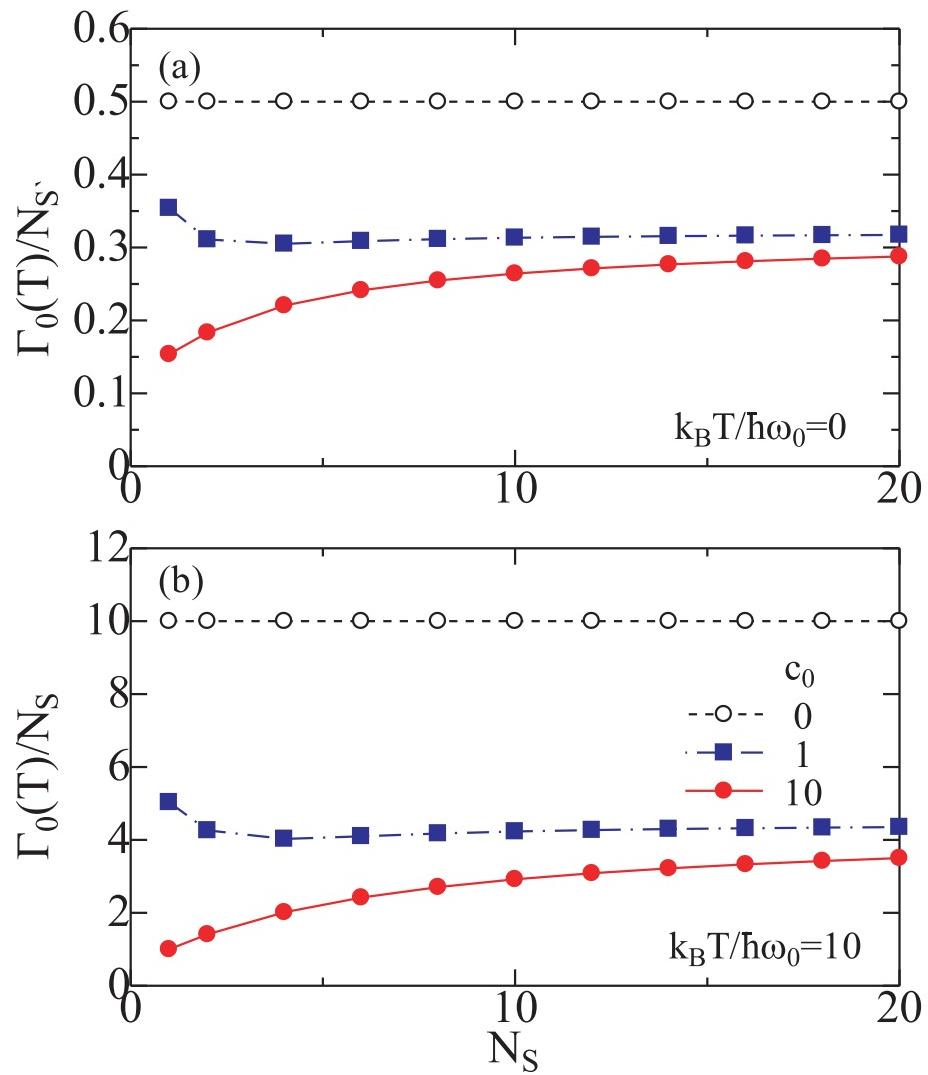


FIG. 8: (Color online) The N_S dependence of $\Gamma_0(T)/N_S$ at (a) $k_B T/\hbar\omega_0 = 0.0$ and (b) $k_B T/\hbar\omega_0 = 10.0$ for $c_0 = 0.0$ (dashed curve), 1.0 (chain curve) and 10.0 (solid curve) of a HO system ($N_S = 10$, $N_B = 100$, $K = D = M = m = \omega_0 = 1.0$).

Acknowledgments

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